Non-Universal Extinction Transition for Boundary Active Site

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We present a generalized model of a diffusion-reaction system where the reaction occurs only on the boundary. This model reduces to that of Barato and Hinrichsen when the occupancy of the boundary site is restricted to zero or one. In the limit when there is no restriction on the occupancy of the boundary site, the model reduces to an age dependent Galton-Watson branching process and admits an analytic solution. The model displays a boundary-induced phase transition into an absorbing state with rational critical exponents and exhibits aging at criticality below a certain fractal dimension of the diffusion process. Surprisingly the behavior in the critical regime for intermediate occupancy restriction N varies with N. In fact, by varying the lifetime of the active boundary particle or the diffusion coefficient in the bulk, the critical exponents can be continuously modified.

Nonequilibrium phase transitions can differ significantly from their equilibrium cousins, and are a subject of continuing interest. Recently, Barato and Hinrichsen [1, 2] (BH) studied a reaction-diffusion model apparently exhibiting a new universality class of nonequilibrium phase transitions, boundary induced phase transitions. The model they studied was a variant of a model introduced earlier by Deloubrière and van Wijland [3], who however did not discover the novel scaling behavior. In this letter we generalize the model and solve it analytically in a certain limit. Our model exhibits a phase transition and at criticality we find the presence of aging [4, 5] , a nonequilibrium property observed in such diverse systems as spin-glasses [4], gels [6] and turbulence [7]. Furthermore a critical fractional dimension for the diffusion process is naturally obtained in the context of our model. Interestingly we find that the critical exponents of the model vary continuously with the parameters of the model. We also note that our toy model is interesting in the context of catalytic reactions and biological situations when the reaction occurs on a specific membrane, such as a boundary of a cell.

Our model is defined as follows: As in the BH model, a particle starting on the boundary follows a birth-death process. It produces an offspring (next to the boundary site) with probability p ($A \xrightarrow{p} A + O$) and dies with probability $1 - p$ ($A \xrightarrow{1-p} \varnothing$). The particle A continues to reproduce until it dies. The offspring O diffuse freely in the bulk since their birth and up to the time they reach the boundary, and then they start to reproduce again according to the same death-birth process. By varying the rate of offspring production, one expects to reach extinction for $p \to 0$ (absorbing state) and a growing or stable population for $p \to 1$, intuitively one expects a transition between those two states as p grows from 0 to 1. In the BH model, there is a constraint that only one particle can exist on the boundary site at any give time. Any other particle trying to enter the boundary site dies immediately. We generalize this to allow up to N particles to coexist simultaneously on the boundary. As shown by BH, the role of the bulk diffusion is just to generate a probability distribution $\psi(t)$ for the arrival of the newly born particle to the boundary site, where it can, if the boundary site is not fully occupied, reproduce some number of times, setting off new processes and then die. Introducing constraints on the occupancy of the bulk sites has no effect on the global dynamics, due to the indistinguishability of different particles [8]. By totally relaxing the constraint on the boundary occupancy, i.e., $N \to \infty$, we are capable of completely solving the model since technically the unrestricted model is a random branching, or Galton-Watson, process.

In the unrestricted case we can make another simplification, since the time to die is governed by a short-range exponential distribution, we can, without doing any harm to the model, consider all births as happening simultaneously. In this view, the particle generates k children, governed by a geometrical distribution, $p_k = (1 - p)p^k$, and then immediately dies. The basic technique employed in the analysis is the use of the generating functional [9] and parallels the solution of the standard age-dependent branching process [10]. Let us denote by $Z(t, t + s)$ the number of particles that been observed on the boundary during the time interval $(t, t + s)$. We define a generating function for the random variable $Z(t, t+s)$ as the average of $s^{Z(t,t+s)}$ over the distribution of $Z(t, t + s)$

$$G_{(t,t+s)}(s) = \sum_{Z(t,t+s)=0}^{\infty} \mathrm{P}(Z(t, t + s))s^{Z(t,t+s)}, \quad (1)$$

where $\mathrm{P}(Z(t, t + s))$ denotes the probability to observe $Z(t, t+s)$ particles on the boundary in the specified time interval. The generating function for the number of offsprings is $G_O(s) = \langle s^k \rangle = (1 - p)/(1 - ps)$. We set the initial conditions such that at $t = 0$ a single particle was injected into the bulk and it has the probability distribution $\psi(t)$ to return to the boundary at time $t = t_R$. By conditioning on the outcome of the returning time

for the first particle [10], we obtain [11] the equation for $G_{(t,t+s)}(s)$

$$G_{(t,t+s)}(s) = \int_0^t G_O(G_{(t-u,t-u+s)}(s))\psi(u)du$$
$$+s\int_t^{t+s} G_O(G_{(0,t-u+s)}(s))\psi(u)du + \int_{t+s}^\infty \psi(u)du. \tag{2}$$

In the limit of $s \to 0$ the generating function goes to $P(Z(t, t + s) = 0) := P_E(t, s)$, i.e. the probability that not a single particle appears on the boundary at the mentioned time interval, taking this limit in Eq. (2) we obtain

$$P_E(t, s) =$$
$$\int_0^t \frac{1-p}{1-pP_E(t-u,s)}\psi(u)du + \int_{t+s}^\infty \psi(u)du, \tag{3}$$

where we have now used the explicit from of $G_O(s)$. Eq (3), a non-linear Volterra equation of the second kind, is our main equation for the unrestricted case of the model and it describes the time evolution of a two-time quantity. We haven't assumed anything as to the form of $\psi(t)$ and so Eq. (3) is quite general. The long-time behavior of P_E is, as we shall see, governed entirely by the long time behavior of $\psi(t)$. For normal diffusion in the bulk, this long-time behavior is $\psi_t \sim \psi_\infty t^{-(1+\beta)}$, with $\beta = 1/2$, $\psi_\infty = 1/\sqrt{4\pi D}$, where D is the diffusion constant (defined as usual). We also consider the more general case of $0 < \beta < 1$, and in such case the constant ψ_∞ is used for the normalization of ψ_t. The case of $0 < \beta < 1$ can be achieved if the diffusion in the bulk is anomalous [12]; e.g., subdiffusion for $0 < \beta < 1/2$ described by models such as the continuous time random walk (CTRW) [12, 13]. Herein we study P_E exclusively; other quantities such as the mean number of particles can also be obtained from Eq. (2) [11].

We will now explore the behavior of $P_E(t, s)$ in the asymptotic limit of large t for different values of the parameters p and β. Inspired by numerical solutions of Eq. (3), we adopt the ansatz

$$P_E(t, s) = P_E^\infty - A(s)t^{-\alpha} \qquad t \to \infty \tag{4}$$

In order to obtain a solution of Eq. (3) we substitute the asymptotic form in Eq. (4) into both sides of Eq. (3), perform an expansion in inverse powers of t and compare the coefficients in front of the appropriate leading terms. We leave the exact technical details for a longer publication [11] and now provide only the final results.

So doing, in the limit $t \to \infty$, s fixed, we obtain

$$P_E^\infty = \begin{cases} \frac{1-p}{p} & p \geq 1/2 \\ 1 & p \leq 1/2 \end{cases} \tag{5}$$

which clearly points out the existence of a critical $p = p_c = 1/2$. The location of the critical point at $p = 1/2$ is due to the fact that at this value, each particle on

the boundary produces exactly one offspring. Below this point, the number of particles decreases exponentially with the number of past boundary particles, and above it it grows exponentially. The behavior of $A(s)$ and α for the off-critical state, $p \neq p_c$, is given by

$$A(s) = \begin{cases} \frac{1-p}{1-2p}\frac{\psi_0}{\beta}s & p < 1/2 \\ -1 & p > 1/2 \end{cases}, \tag{6}$$

$$\alpha = \begin{cases} 1+\beta & p < 1/2 \\ \beta & p > 1/2 \end{cases}. \tag{7}$$

The presence of the phase transition as we approach $p = 1/2$ from below is clearly manifest in the divergence of the coefficient A. The approach from above is not obvious from the large t behavior. What happens is that for $p \gtrsim 1/2$, P_E first rises toward unity, as happens below the transition. However, at very large t, the behavior crosses over toward the power-law decay toward P_E^∞. The details of this crossover will be presented in our longer presentation [11].

In the critical state, $p = p_c$ Eq. (5) remains valid and so $P_E^\infty = 1$ while the behavior of $A(s)$ and α shows a transition as a function of β. For α, we obtain

$$\alpha = \begin{cases} 1-\beta & \beta \leq 1/2 \\ \beta & \beta \geq 1/2 \end{cases}, \tag{8}$$

We can exhibit an analytic expression for $A(s)$ at p_c only for $\beta > 1/2$:

$$A(s) = -\frac{\pi\csc(\beta\pi)\Gamma(1-b)}{\Gamma(1-2\beta)\Gamma(1+\beta)} \qquad (\beta > 1/2) \tag{9}$$

For $\beta < 1/2$, $A(s)$ has to be calculated numerically in general. However, in the limit of large s, we have

$$A(s) \propto s^{1-\beta} \qquad (\beta < 1/2). \tag{10}$$

The existence of a special β for the behavior at criticality is very non-trivial and it is especially interesting that the critical β_c is equal to $1/2$, i.e the normal diffusion case. We can treat this critical β_c as a critical fractal dimension since 2β is just the fractal dimension of the diffusion. For the special case of $\beta = 1/2$ our ansatz, i.e. Eq. (4), does not work and one needs to treat this case specially [11]; the result is

$$1 - P_E(t, s) \propto \frac{1}{\log(s/t)}\left(s/t\right)^{1/2} \qquad (\beta = 1/2). \tag{11}$$

The logarithmic corrections in the behavior support our claims as to the critical nature of $\beta = 1/2$. For a two time quantity like the survival probability $P_S(t, s) = 1 - P_E(t, s)$, one usually expects for a stationary process a dependence only on the time difference s; when the process is non-stationary this is generally not true. When the time dependence is that of a ratio of the two

times this is usually defined as aging, as in our case $P_S(t, s) \propto (s/t)^{1-\beta}$. The aging behavior for $\beta \leq 1/2$ at criticality is a signature of the nonequilibrium phase transition properties, which have been studied extensively in the context of DP and Contact Process [5, 14, 15], and the nonstationarity of the process usually obtained in glassy dynamics [4]. We must note that the obtained result where the probability to observe at least one particle in time interval s is proportional to $s^{1-\beta}$ ($\beta < 1/2$) is unexpected in light of the fact that for the off-critical state ($p < p_c$), this probability is proportional to s.

Now we treat the limit $s \gg t \gg 1$, where we take first $s \to \infty$. In this limit we can neglect the second term on the right hand side of Eq. (3) and define $P_E(t, \infty) = P_E(t)$ simply as the extinction probability of the process. We are now dealing with a single-time quantity and so no aging behavior could be obtained. For the solution we use the same ansatz as in Eq. (4), writing $A(\infty) = A$. The equation for P_E^∞ remains the same as Eq. (5) and one again obtains the same critical value for p, $p_c = 1/2$. In the off-critical state the results for α and A are

$$\alpha = \beta, \tag{12}$$

and

$$A(s) = \begin{cases} \frac{1-p}{1-2p} \frac{\psi_0}{\beta} & p < 1/2 \\ \frac{1-p}{1-2p} \frac{\psi_0}{\beta} & p > 1/2 \end{cases}. \tag{13}$$

The transition in this limit is different then in the previously discussed limit of $t \gg s$, as A diverges similarly near p_c and thus describes the crossover time scale on which one would observe critical behavior. For the critical state $p = p_c$ we obtain

$$P_E(t) \sim 1 - \left(\frac{\psi_0}{\beta}\right)^{\beta/2} t^{-\beta/2}. \tag{14}$$

Thus for the survival probability of the process, $P_S(t) = 1 - P_E(t)$, we obtain the power-law behavior $P_S(t) \sim t^{-\delta}$ with $\delta = \beta/2$. The special properties of $\beta = 1/2$ are not observed in the limit of $s \gg t$, and as already been mentioned no aging behavior could be observed for a one-time quantity. The noncomutativity of the limits $t \to \infty$ - $s \to \infty$ is similar in some sense to the non commutativity of the same limits present for correlation function behavior in glassy systems [4] and leads to such non-equilibrium property as ergodicity breaking [16, 17]

Thus, in the case of normal diffusion, i.e. $\beta = 1/2$, for our modified model with unrestricted occupation of the origin, we have a phase transition at $p = 1/2$ with a critical exponent for the survival probability of $\delta = 1/4$, observed also in numerical simulations [2] . This is in contrast with the original model, with a larger critical p, but more importantly, a survival exponent of $\delta \approx 0.17$. The change in the phase transition point is clear, since in the original $N = 1$ model, some children die upon their
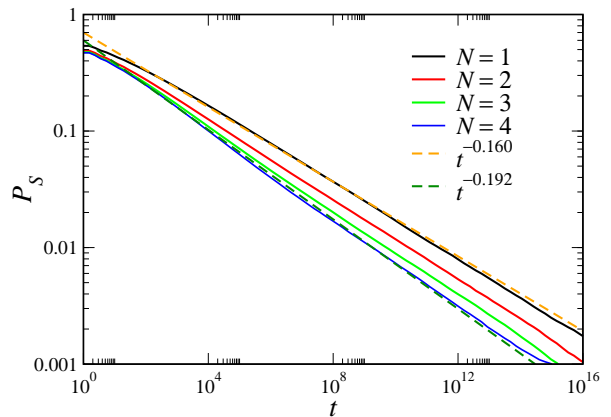

FIG. 1: The survival probability vs. time for $N = 1, 2, 3$, and 4, together with power-law fits for the cases $N = 1$ and $N = 4$.

attempted return to the origin and so the critical p has to be larger than $1/2$ to compensate. The change in exponent is not unexpected. For directed percolation, the critical exponents in a model of unrestricted occupancy are the mean-field exponents, which differ from the exponents in the restricted occupancy version[18].

In the case of directed percolation, for any finite N the critical exponents are those of the $N = 1$ model. For large N, there is a crossover in the scaling between the mean-field scaling of the $N = \infty$ model and the directed percolation exponents [18]. Based on this analogy, one would expect a similar behavior in the present case, with the critical behavior for any finite N being identical to the $N = 1$ model.

To test this hypothesis, we have measured the survival exponent δ at criticality for various N. The results are shown in Fig. 1. We see that, contrary to our naive expectation, there is a different exponent for each N. The measured best fit exponents are, for example, $\delta = 0.160$ for $N = 1$, $\delta = 0.171$ for $N = 2$, $\delta = 0.180$ for $N = 3$ and $\delta = 0.192$ for $N = 4$. There is no sign of any crossover behavior. One test for this is shown in Fig. 2, where we show $P_S(t) t^\delta$, in a linear(y)-log(x) scale. We see that the graphs all exhibit the same characteristic oscillation in $\ln(x)$ [19] that makes accurate determination of an exponent so difficult, but they show no secular trend.

Varying N is not the only way to interpolate between the two models and thereby vary δ. We can instead introduce a parameter Δ which controls the lifetime of a particle on the active site after reproduction (in the original model, $\Delta = 1$). As Δ decreases, the interference between different particles is reduced, and the theory approaches the noninterference, Galton-Watson, limit. We can also
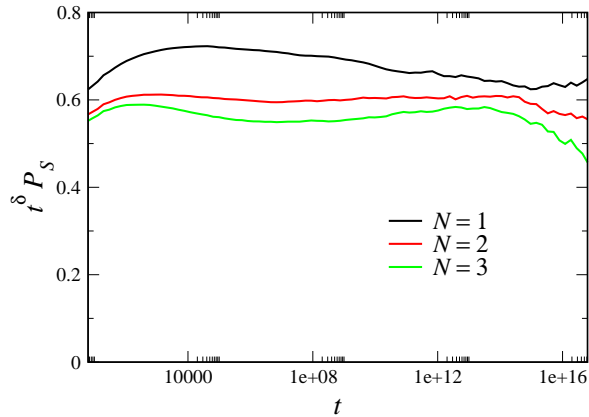
FIG. 2: The survival probability, P_S^N, multiplied by $e^{\delta_N t}$ as a function of time for $N = 1$, 2 and 3. The values of δ_N are as noted in the text.

FIG. 3: The measured survival exponent δ as a function of Δ, the lifetime of the particle on the active site after it gives birth. The simulations were performed for measurement time $t \sim 10^{16}$.

increase Δ beyond one, and make the interference effect stronger, thereby reducing the exponent below the original BH value. Actually the precise dimensionless parameter which controls the exponent δ is $\Delta/\psi_\infty^2 \propto D\Delta$, which presents a surprising dependence of the critical exponent δ on the diffusion coefficient (D) in the bulk. This is demonstrated in Fig. , where the survival exponent is plotted as a function of Δ. We see that as opposed to the discrete parameter N, now the exponent varies continuously, decreasing with $D\Delta$.

Finally we note that the relevance of the limit for which we managed to solve the model analytically is much broader when one considers higher dimension systems. We have studied herein a one dimensional system where the boundary is zero dimensional, while if one considers a d dimensional system where the boundary is of dimension $d-1$, a line or a membrane, in such a case even if $D\Delta$ does not approach zero, the probability that two particles would try to occupy the same site (since there an infinite number of sites on boundary) during the time $D\Delta$ is small and this would lead to a larger applicability of our analytical solution. Another type of system where our results could be applied is systems with anomalous diffusion behavior described by the Continuous Time Random-Walk model [13], for such systems the results stays valid even if the size of the system is finite as for a finite system with regular diffusion our results are modified for times long enough [11].

In summary, we have extended to finite active site occupancy N and solved analytically the $N \to \infty$ limit of the Barato-Hinrichsen model, yielding the scaling exponents of the extinction transition in this limit. We have also show that below a critical fractal dimension for the
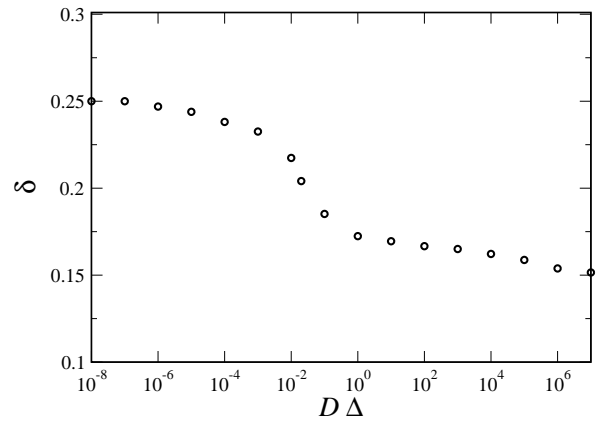
diffusion process in the bulk, there is aging behavior at the transition. In addition, we have seen that the exponents are in fact not universal, varying with N or the scaled lifetime of the particles on the active site. This is of course very different from the situation that obtains in the superficially similar contact process, which exhibits universal Directed Percolation scaling.

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